

2,3-O-Isopropylideneerythrose
37669-01-5 | DTXSID60191084

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 77.1 °C

Global applicability domain: Inside

Local applicability domain index: 4.45e-01

Confidence level: 5.39e-01

Nearest Neighbors from the Training Set

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4-Hydroxy-2,5-dimethyl-
3(2H)furanone
Measured: 80.5
Predicted: 78.8

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5-(Hydroxymethyl)-2-furfural
Measured: 31.5
Predicted: 72.6

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Isomaltol
Measured: 100
Predicted: 80.5

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Penicillic acid
Measured: 83.0
Predicted: 70.6